- (1) Decane; C₁₀H₂₂; [124-18-5]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

CRITICAL EVALUATION:

Quantitative solubility data for the decane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Decane (1) - Water (2) System

Reference T/K Solubil	ity Method
Baker (ref 1,2) 298 (1) in	(2) radiotracer
Schatzberg (ref 3) 298,313 (2) in	(1) Karl Fischer
Franks (ref 4) 298 (1) in	(2) GLC
McAuliffe (ref 5) 298 (1) in	(2) GLC
Krasnoshchekova and 298 (1) in Gubergrits (ref 7)	(2) GLC
Mackay et al . (ref 8) $-a$ (1) in	(2) GLC
Namiot <i>et al.</i> (ref 9) $423-583^{b}$ (2) in	(1) vapliq.equil.
Skripka (ref 10) $398-563^{b}$ (2) in	(1) vapliq.equil.
Becke and Quitzsch (ref 11) 293 mutua	l refractometric

 $[\]alpha$ Not specified but probably 298.15K.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition, Roof (ref 6) has reported a three phase critical point of unknown composition at 569K and 9.6 MPa. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF DECANE (1) IN WATER (2)

The available data on the solubility of decane in water are summarized in Table 2 with the following exceptions. The value of Baker in ref 2 is quoted in v/v terms and is therefore excluded from consideration (however it is equivalent to that reported by the same author in ref 1). The values of Mackay et al. (ref 8) are rejected not only because the measurement temperature was unspecified but also because the authors themselves regard their solubility values below 2 x 10^{-3} g(1)/100g sln as potentially unreliable because of emulsion or colloid formation. The value of McAuliffe (ref 5) is also rejected because it is very much higher than all other reported values.

Agreement among the remaining values (Table 2) is not good enough to enable any of the "Best" values to be Recommended.

(continued next page)

b Pressure also varied 1-78 MPa.

COMPONENTS:	EVALUATOR:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Water; H ₂ O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of Decane (1) in Water (2)

T/K	Solubility values		
	Reported values $10^6 ext{g(1)/100g sln}$	"Best" valu 10 ⁶ g(1)/100g sln	
293	1.98 (ref 11)	2	2.5
298	1.6 (ref 1), 1.98 (ref 4), 0.87 (ref 7)	1.5 ± 0.5	1.9

 $[\]alpha$ Obtained by averaging; $\sigma_{\mbox{\scriptsize n}}$ has no statistical significance.

2. SOLUBILITY OF WATER (2) IN DECANE (1)

At atmospheric pressure the only available values of the solubility of water in decane are those of Schatzberg (ref 3) and Becke and Quitzsch (ref 11). These data are listed in Table 3 but are in poor agreement and can only be regarded as order of magnitude values.

At higher temperatures and pressure only the data of Skripka and co-workers (ref 9,10) are available and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheets for the experimental values.

TABLE 3: Approximate Solubility Values of Water (2) in Decane (1)

T/K	Reported values a		
	10 ² g(2)/100g sln	10 ³ x ₂	
293	2.92 (ref 11)	2.3	
298	0.72 (ref 3)	0.6	
313	1.36 (ref 3)	1.1	

lpha Values considered as order-of-magnitude data only, see text.

REFERENCES

- Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints 1958, 3, No.4, C61-8.
- 2. Baker, E.G. Science 1959, 129, 871-4.
- 3. Schatzberg, P. J. Phys. Chem. <u>1963</u>, 67, 776-9.

(continued next page)

- (1) Decane; C₁₀H₂₂; [124-18-5]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch

University, Perth, W.A., Australia.

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

- 4. Franks, F. Nature 1966, 210, 87-8.
- 5. McAuliffe, C. Science 1969, 163, 478-9.
- 6. Roof, J.G. J. Chem. Eng. Data 1970, 15, 301-3.
- Krasnoshchekova, P.Y.; Gubergrits, M.Y. Neftekhimiya 1973, 13, 885-7.
- 8. Mackay, D.; Shiu, M.W.; Wolkoff, A.W. Water Quality Parameters, ASTM STP 573, 1975, 251-8.
- 9. Namiot, A.Y.; Skripka, V.G.; Lotler, Y.G. Zh. Fiz. Khim. 1976, 50, 2718; Deposited doc. 1976; VINITI 1213-76.
- Skripka, V.G. Tr. Vses. Neftegazov. Nauch-Issled. Inst. 1976, 61, 139-51.
- 11. Becke, A.; Quitzsch, G. Chem. Techn. 1977, 29, 49-51.

- (1) Decane; C₁₀H₂₂; [124-18-5]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Baker, E.G.

Am. Chem. Soc., Div. Petrol.
Chem., Preprints 1958, 3, N°4,
C61-8.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of decane-1- C^{14} in water at 25°C was reported to be 16 x 10^{-9} g(1)/g(2).

The corresponding mole fraction, calculated by the compiler, is $x_1 = 2.0 \times 10^{-9}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Carbon-14 labeled (1) was used as radioactive tracer. The technique of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)-(2) dispersion has been described in ref 1. A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dissolved in (2).

SOURCE AND PURITY OF MATERIALS:

- Nuclear Instrument and Chemical Corporation; used as received.
- (2) distilled.

ESTIMATED ERROR:

REFERENCES:

 Baker, E.G. Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia 1956, 1, N°2, 5.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5]	Baker, E.G.
(2) Water; H ₂ O; [7732-18-5]	Science 1959, 129, 871-4.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	F. Kapuku
EXPERIMENTAL VALUES:	
	25°G was reported to be
The solubility of decane in water at 22×10^{-7} mL(1)/100 mL(2).	25°C was reported to be
(2), 200	
	ļ
ATIVITITADV	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
not specified.	not specified.
	1
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

- (1) Decane; C₁₀H₂₂; [124-18-5]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schatzberg, P.

J. Phys. Chem. 1963, 67, 776-9.

VARIABLES:

PREPARED BY:

Temperature: 25-40°C

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in decane

t/°C	mg(2)/kg sln	<u>*2</u>
25	72 ^a	5.7×10^{-4}
40	136 ^b	10.7×10^{-4}

a,b See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

- (1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydro-phobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.
- SOURCE AND PURITY OF MATERIALS:
 - (1) Phillips Petroleum Co.; research grade; 99.43 mole%; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.
- (2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02°C

soly. a) 0-6%; b) 0-2% (deviations from the mean)

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Decane; C₁₀H₂₂; [124-18-5] Franks, F. Nature (London) 1966, 210, 87-8. (2) Water; H₂O; [7732-18-5] VARIABLES: PREPARED BY: F. Kapuku One temperature: 25°C

EXPERIMENTAL VALUES:

The solubility of decane in water at 25°C was reported to be in mole fraction $x_1 = 2.5 \times 10^{-9}$. The corresponding mass percent calculated by the compiler is

 $1.98 \times 10^{-6} \text{ g(1)/100 g sln.}$

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 ml of the aqueous phase was injected into the fractionator fitted to the chromatographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.

SOURCE AND PURITY OF MATERIALS:

- (1) Fluka; purum grade;
 purity > 97% (chromatographic analysis).
- (2) not specified.

ESTIMATED ERROR:

soly. ± 12%

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Decane; C₁₀H₂₂; [124-18-5] McAuliffe, C. (2) Water; H₂O; [7732-18-5] Science 1969, 163, 478-9. VARIABLES: PREPARED BY: One temperature: 25°C F. Kapuku

EXPERIMENTAL VALUES:

The solubility of decane in water at 25°C was reported to be 0.052 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 5.2 x 10^{-6} g(1)/100 g sln and 6.58 x 10^{-9} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

- (1) was equilibrated with (2). Glass (1) not specified. Vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaken for 2 minutes. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.
- SOURCE AND PURITY OF MATERIALS:
 - (2) distilled.

ESTIMATED ERROR:

soly. \pm 0.0043 mg(1)/kg(2)

- (1) Decane; C₁₀H₂₂; [124-18-5]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Krasnoshchekova, P.Ya.; Gubergrits, M.Ya.

Neftekhimiya 1973, 13, 885-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of decane in water at 25°C was reported to be $x_1 = 1.1 \times 10^{-9}$.

The corresponding mass percent calculated by the compiler is 8.7×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigor-ously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.

SOURCE AND PURITY OF MATERIALS:

- (1) source not specified; CP reagent; purity not specified.
- (2) distilled.

ESTIMATED ERROR:

not specified.

COMPONENTS: (1) Decane; C₁₀H₂₂; [124-18-5] (2) Water; H₂O; [7732-18-5] VARIABLES: not specified ORIGINAL MEASUREMENTS: Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. 1975, 573, 251-8. PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported two different values for the solubility of decane in water: 0.182 and 1.22 mg(1) dm⁻³ sln. With the assumption of a solution density of 1.00 g cm⁻³, the corresponding mass percents calculated by the compiler, are 0.0000182 and 0.000122 g(1)/100 g sln and the corresponding mole fractions, x_1 , are 2.3 x 10^{-8} and 1.6 x 10^{-7} respectively.

AUXILIARY INFORMATION

(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equilibrations it is possible to calculate the amount of (1) in the original sample.

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

- (1) not specified.
- (2) not specified.

ESTIMATED ERROR:

not estimated.

- (1) Decane; C₁₀H₂₂; [124-18-5]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Namiot, A.Yu.; Skripka, V.G.; Lotter, Yu.G.

Zh. Fiz. Khim. 1976, 50, 2718 Deposited doc. 1976, VINITI 1213-76.

VARIABLES:

Temperature: 150-310°C Pressure: 0.52-8.44 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in decane

t/°C	p/kg cm ⁻²	<pre>p/MPa (compiler)</pre>	*2 —	g(2)/100 g sln (compiler)
150	5.3	0.52	0.028	0.36
200	18.2	1.79	0.095	1.31
225	30	2.9	0.162	2.39
250	47.2	4.63	0.248	4.01
275	73.2	7.18	0.403	7.87
285	83.9	8.23	0.504	11.4
290	95.4	9.36	0.606	16.3
310	20	2.0	0.029	0.38
310	30	2.9	0.069	0.93
310	40	3.0	0.114	1.60
310	50	4.9	0.171	2.54
310	60	5.9	0.239	3.82
310	70	6.9	0.313	5.45
310	80	7.8	0.407	7.99
310	86.1	8.44	0.520	12.06

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The static method for vapor-liquid equilibrium described in ref 1 was used.

No more details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

- (1) source not specified; CP reagent; used as received.
- (2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

 Sultanov, R.G.; Skripka, V.G.; Namiot, Yu.A. Zh. Fiz. Khim. 1976, 46, 2170.

COMPONENTS: (1) Decane; C₁₀H₂₂; [124-18-5] (2) Water, H₂O; [7732-18-5] Skripka, V.G. Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, 61, 139-51. Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. 1973, 47, 1035.

VARIABLES: Temperature: 225-290°C Pressure: 2.9-78.5 MPa PREPARED BY:

A. Maczynski

XPERIMENTA	Solub	ility of water in	decane	
t/°C	p/kg cm ⁻²	<pre>p/MPa (compiler)</pre>	*2 	g(2)/100 g sln (compiler)
225	30	2.9	0.162	2.39
	50	4.9	0.157	2.30
	70	6.9	0.153	2.28
	100	9.8	0.148	2.15
	150	14.7	0.138	1.99
	200	19.6	0.132	1.89
	250	24.5	0.124	1.76
	300	29.4	0.118	1.67
	400	39.2	0.108	1.51
	500	49.0	0.102	1.42
	600	58.8	0.098	1.36
	700	68.6	0.095	1.31
	800	78.5	0.094	1.30
250	50	4.9	0.255	4.15
	70	6.9	0.248	4.01
	100	9.8	0.240	3.84
	150	14.7	0.226	3.56
	200	19.6	0.213	3.31
	250	24.5	0.200	3.07
	300	29.4	0.190	2.88
	400	39.2	0.168	2.49
	500	49.0	0.158	2.32
	600	58.8	0.153	2.24
	700	68.6	0.151	2.20
	800	78.5	0.148	2.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental technique was described in ref 1. No details reported in the paper.

SOURCE AND PURITY OF MATERIALS:

- (1) source not specified, chemical reagent grade; purity not specified; used as received.
- (2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

 Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. Gazov. Prom. 1971, 4, 6.

(2) Water; H₂O; [7732-18-5]

(1) Decane; C₁₀H₂₂; [124-18-5] Skripka, V.G. Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, 61, 139-51.

Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. 1973, 47, 1035.

t/°C	p/kg cm ⁻²	<pre>p/MPa (compiler)</pre>	<i>x</i> ₂	g(2)/100 g sln (compiler)
275	70	6.9	0.404	7.90
	100	9.8	0.385	7.34
	150	14.7	0.353	6.46
	200	19.6	0.320	5.62
	250	24.5	0.293	4.98
	300	29.4	0.272	4.52
	400	39.2	0.246	3.97
	500	49.0	0.231	3.66
	600	58.8	0.217	3.39
	700	68.6	0.204	3.14
	800	78.5	0.197	3.08
290	100	9.8	0.580	14.88
	150	14.7	0.417	8.30
	200	19.6	0.392	7.54
	250	24.5	0.371	6.95
	300	29.4	0.350	6.38
	400	39.2	0.318	5.57
	500	49.0	0.291	4.94
	600	58.8	0.270	4.47
	700	68.6	0.253	4.11
	800	78.5	0.243	3.90

COMPONENTS: (1) Decane; C₁₀H₂₂; [124-18-5] (2) Water; H₂O; [7732-18-5] VARIABLES: One temperature: 20°C ORIGINAL MEASUREMENTS: Becke, A.; Quitzsch, G. Chem. Techn. 1977, 29, 49-51.

EXPERIMENTAL VALUES:

The solubility of decane in water at 20°C was reported to be in mole fraction, $x_1 = 2.5 \times 10^{-9}$. The corresponding mass percent, calculated by the compiler, is 1.976×10^{-6} g(1)/100 g sln. The solubility of water in decane at 20°C was reported to be in mole fraction, $x_2 = 2.3 \times 10^{-3}$. The corresponding mass percent, calculated by the compiler, is 0.0292 g(2)/100 g sln.

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The refractometric and the KarlFischer dead-stop titration methods were used. No more details are given in the paper. ESTIMATED ERROR: soly. 0.05-1% for (1) in (2) 0.3-1.3% for (2) in (1) REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

CRITICAL EVALUATION:

The solubility of decane (1) in seawater (2) has been reported in two works:

Authors	Method	<u>T/K</u>	Salinity g salts/kg sln	g(1)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	298	6	8.7×10^{-6}
Freegarde et al. (ref 2)	GLC	?	?	1.5×10^{-5}

Because temperature and salinity are not specified, the data of Freegarde $et\ al.$ are rejected. The value of Krasnoshchekova and Gubergrits is considered doubtful since it is greater than the tentative value for the solubility of decane in pure water at 298 K.

SOLUBILITY OF DECANE (1) IN SEAWATER (2) DOUBTFUL VALUE

T/K	g salts/kg sln	g(1)/100 g sln
298	6	8.7×10^{-6}

- Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. Neftekhimiya 1973, 13, 885-8.
- Freegarde, M.; Hatchard, C.G.; Parker, C.A. Lab. Pract. 1971, 20, 35-40.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Seawater (composition not specified)	Freegarde, M.; Hatchard, C.G.; Parker, C.A. Lab Pract. 1971, 20, 35-40.
VARIABLES:	PREPARED BY:
Temperature, pressure, salinity not given.	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of decane was reported to be 0.15 mg/L. The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 1.5 x 10^{-5} g(1)/100 g sln and 1.9 x 10^{-8} , assuming a solution density of 1.02 kg/L.

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: None given except that analysis was done using gas chromatography. ESTIMATED ERROR: not specified. REFERENCES:

- (1) Decane; C₁₀H₂₂; [124-18-5]
- (2) Seawater

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.; Gubergrits, M.Ya.

Neftekhimiya 1973, 13, 885-8.

VARIABLES:

One temperature: 25°C Salinity: 6 g/kg sln

PREPARED BY:

M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of decane in seawater was reported to be 8.7 x 10^{-6} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 1.1 \times 10^{-8}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

SOURCE AND PURITY OF MATERIALS:

- (1) "chemically pure"
- (2) distilled water plus salt mixture.

ESTIMATED ERROR:

not specified.